The Modelling of the Particle/Turbulence Interaction for
Oil and Coal- Fuelled Combustors

F.C. Lockwood, C. Papadopoulos and S.A.L. Perera
Department of Mechanical Engineering,
Imperial College of Science, Technology and Medicine,
London SW7 2AZ, United Kingdom.

Key words: Particle dispersion, correlation coefficient, evolving probability

INTRODUCTION

Most of the existing predictive codes rely on a stochastic treatment of the particle-turbulence interaction in which the trajectories of particles of finite number of representative sizes emerging from representative starting locations are computed. To obtain statistically reasonable results for position and velocity probability density functions(pdfs), more than 1000 particles from each size group and starting location must be tracked, thus they are not attractive in terms of computer economy.

The "Prediction of Evolving Probability(PEP)" model is a novel method developed by Lockwood and Papadopoulos[5] to predict the evolution in time of the particles velocity pdf for two-phase flows. Given the gas conditions at the current particle position, the model predicts the particles velocity pdf for the chosen time step which gives the particle position.

In the present work PEP model is incorporated in the 2D-code FAFNIR in which the treatment of gas phase is based on the standard k-ε model. The calculation of the turbulent flow with the dispersed particulate phase is based on a statistically steady Eulerian framework for the motion of the carrier continuum phase and a Lagrangian simulation of the particulate phase.

Gas Flow Field

The gas flow is described by transport equations for mass, momentum and turbulence quantities which can be cast in the general form applicable to 2D, steady, non swirling, axisymmetric geometries:

$$\frac{\partial}{\partial x_i}(\rho U_i \phi) = \frac{\partial}{\partial x_i}\left(\Gamma_{eff}\frac{\partial \phi}{\partial x_i}\right) + S_\phi + S_\phi^P \qquad [1]$$

where U_i is the velocity component in direction x_i, the implied summation being restricted to the axial and radial components; ϕ represents any of the variables U,V,k,ε or h. The S_ϕ and Γ_{eff} are, respectively, the 'source' and the effective diffusion coefficients for the entity ϕ, while S_ϕ^P represents the particular source due to the presence of the particulate phase. The continuity equation is obtained by setting ϕ=1 and Γ_{eff}=1.

The interaction with the dispersed particulate phase which is represented by S_ϕ^P is obtained using the 'Particle Source in Cell(PSIC)' method, Crowe et al[1], where the cells are the finite difference control volumes of the discretised flow domain for the gas phase calculation. These terms are calculated by the integration of all particle trajectories crossing a given control volume. The turbulence scales k and ε are obtained using the standard k-ε model equations and constants, Launder and Spalding[4].

Particle Flow Field

The Lagrangian form of the governing equations for the particulate phase are analytically solved to predict the evolution in time of the particles velocity pdf. The instantaneous acceleration of a particle immersed in a gas at time t, in its non-linearised form, may be expressed as:

$$\frac{du_p(t)}{dt} = \frac{\rho_g A_p C_D}{2m_p} SIGN[u_g(t)-u_p(t)]^2 + Fp \qquad [2]$$

The particle drag coefficient, C_D, in general is a function of the Reynolds number based on gas-particle relative velocity. The following drag law has been employed for the present study.

$$C_D = \left(1.0+0.15Re_p^{0.687}\right)/(Re_p/24) \qquad \text{for } Re_p \le 1000$$
$$C_D = 0.44 \qquad \text{for } Re_p > 1000$$

SIGN signifies the sign of the relative velocity of the particle with respect to the gas. F_p is the sum of all forces acting on the particle excluding viscous force expressed by the first term on the right hand side. Only the viscous term is retained for the present formulation which neglect the following:

1.Inertial apparent force and Basset force.
2.Static pressure gradient force in the direction of motion.
3.Buoyancy effects.
4.Magnus effect as the particles are assumed to be non-rotating.

5.Particle-particle interaction.

With a closure assumption that the pdf of the gas velocities is Gaussian given that the pdf for the particle velocity is also Gaussian for the same spatial position and time, see Snyder and Lumley[6], Wells and Stock[9] and Tsuji and Morikawa[7], the equation for the pdf of the ensemble particle velocity at time t, $P(v_p,t)$ is derived as, Lockwood and Papadopoulos[5]:

$$C[C_1+C_2v_p+C_3v_p^2]P_{v_p}+P_t+C[C_2+2C_3v_p]P = 0 \qquad [3]$$

where

$$C = \frac{\rho_g A_p C_D SIGN}{2m_p},$$

$$C_1 = \sigma_g^2(1-\rho_{gp}^2) + \left(\overline{u}_g - \frac{\rho_{gp}\sigma_g}{\sigma_p}\overline{u}_p\right)^2,$$

$$C_2 = 2\left(\overline{u}_g - \frac{\rho_{gp}\sigma_g}{\sigma_p}\overline{u}_p\right)\left(\frac{\rho_{gp}\sigma_g}{\sigma_p} - 1\right),$$

$$C_3 = \left(\rho_{gp}\frac{\sigma_g}{\sigma_p} - 1\right)^2.$$

P stands for the pdf $P(v_p,t)$ and the subscripts v_p and t denote the partial derivatives with respect to the subscripts. σ is the standard deviation of velocity fluctuations and subscripts g and p refers to gas and particulate phases respectively. v_p denotes the particle velocity in probabilistic space while u_g and u_p denote the mean values of velocity in real space. ρ_{gp} is the correlation coefficient for the gas-particle velocity fluctuations.

The solution of the equation [3] using method of characteristics is given by

$$P(v_p;t) = P_0\left[\frac{q^{0.5}}{2C_3}\tan\left(\tan^{-1}\frac{2C_3v_p+C_2}{q^{0.5}} - \frac{Cq^{0.5}t}{2} - \frac{C_2}{2C_3}\right)\right]\frac{\left[\cos\left(\tan^{-1}\frac{2C_3v_p+C_2}{q^{0.5}}\right)\right]}{\left[\cos\left(\tan^{-1}\frac{2C_3v_p+C_2}{q^{0.5}} - \frac{Cq^{0.5}t}{2}\right)\right]} \qquad [4]$$

where $P_O(......)$ stands for the particle velocity pdf at time t=0.

Solution Procedure

Turbulent dispersion of the particles is simulated by sampling the gas phase properties at the current particle position at the beginning of each time step. The fluctuating component of the sampled gas velocity is assumed to be Gaussian with zero mean, for which the standard deviation is given by $\sigma_g=\sqrt{2k/3}$, Gosman and Ioannides[2], where k is the turbulent kinetic energy.

The fluctuating component of the particulate velocity is also treated in a similar manner where the mean particle velocity and its standard deviation are either known as initial conditions or taken from the previous iteration.

The velocity distributions for both the gas and particulate phases are generated analytically at the beginning of each time step with a range of 8σ, Papadopoulos[8]. The range of the most probable particle velocities is discretised into a number of regions of equal width, 20 in the present study, and a representative velocity is assigned to each division. At the end of the time step, values of the evolved representative velocities are sorted with the associated pdf values and these new values are used to calculate the moments of the new particle velocity distribution.

The overall solution procedure for the fluid flow and the particle phase is as follows:

1.A converged solution of the of the gas flow field is calculated without the source terms of the dispersed phase.

2.Representative parcels of particles starting from a finite number of starting locations are traced through the flow field to obtain the mean trajectories and source terms.

3.The flow field is recalculated by considering the source terms of the dispersed phase, where appropriate considering the underrelaxation factors.

4.Repetition of steps 2 and 3 until convergence is reached.

Results and Discussion

Particle motion in a laminar flow is a special case where the gas-particle velocity correlation coefficient and the root mean square(rms) value of the velocity fluctuations are zero, thus giving a simplified solution of the equation [4].

Figure 1 presents the development of the particle velocity in a uniform laminar flow field of mean velocity 10.0m/s. Initial mean particle velocity and its rms value are assumed to be 9.0m/s and

0.5m/s respectively. The rms value of the initial Gaussian distribution of particle velocity diminishes with time to approache a delta function at longer times centred as expected on the mean gas velocity.

Figure 2 shows the turbulent response of three particle size groups 15μm, 40μm and 100μm respectively. The special analytical solution of the equation [4] is used for the case of $\rho_{gp}=1.0$. A free turbulent jet of mean exit velocity 10.0m/s and rms value 0.4m/s is used. Initial mean particle axial velocity and its rms value are assumed to be 9.0m/s and 0.5m/s respectively for all three size groups. It is evident from the figures, that smallest size group tend to follow the mean gas motion whereas the high inertia of the 100μm particles shows a slower response.

On the basis of the evidence presented above and the other supporting evidence by Lockwood and Papadopoulos[5], the PEP model may be applied to a real physical flow field for which experimental data exist.

Detailed measurements of particle dispersion in a round free jet constitutes a reliable reference for validation of a particle dispersion model because gas velocity profiles and turbulent properties can be simulated accurately with the standard k-ε model. Hardalupas et al[9] provides useful measurements for the gas and particulate phases in a round free jet. In the present study, velocity predictions using the PEP model are compared with the experimental measurements, taken using a phased-LDA, for a round, unconfined two-phase jet flow reported by Hardalupas et al[9].

A downward directed jet, exhausting into ambient air environment is used. The flow develops in a 15mm diameter precision bore stainless steel tube for 50mm before exhausting into ambient air.

Due to symmetry, only a half of the flow field is considered. A computational area of 0.5m in radius and 3m in length [Figure 3] with a non-uniform grid of 37*51 is used to simulate the flow field. Outside the injection pipe, the entrainment air flow is initialised to a low velocity, sufficient to prevent recirculation within the flow field.

According to the measurements, the initial velocity of the particles is set to 90% of the mean jet gas exit velocity of 13.1m/s. Particles of 40μm diameter and 2420kg/m^3 density are released from 10 radial positions at the exit of the injection pipe. The jet exit Reynolds number is 13000 with a mass loading of 13%.

Figure 4 shows the centreline variation of the mean axial velocity and its rms value for the particulate phase. Figure 5 presents the radial profiles of the mean particle axial velocity at three axial stations. Predictions using the PEP model with gas-particle velocity correlation coefficient values of 0.1, 0.5 and 1.0 are tested. A gas-particle velocity correlation coefficient of 1.0 gives better overall predictions although the dispersion effect is underpredicted. Considering the results at the first axial station(x/d=10), it is evident that a low correlation coefficient value near the jet exit region gives a much better responce to turbulence.

Figure 6 presents a comparison between the performance of the PEP model with that of a stochastic model similar to one uesd by Gosman and Ioannides[2]. With stochastic model 25 stochastic trials are performed for each particle group. It is clear that the radial profiles of mean axial velocity and its rms value are better predicted by the PEP model with a correlation coefficient of 1.0, although the dispersion is underpredicted. Under prediction of the dispersion can be directly attributed to the use of a constant correlation coefficient value for the whole flow domain at the present state. Analytical determination of the gas-particle correlation coefficient at each sampling location may lead to much superior predictions, but this matter is beyond the scope of the present paper.

A test simulation has been performed imposing an arbitrary linear variation on the value of the correlation coefficient. It is set to 0.2 at the jet exit and increased linearly with axial position to 1.0 at x/d=25 and then allowed to remain constant. As expected, the dispersion effect is clearly improved[Figure 7].

CONCLUSIONS

The effective coding of the PEP model is successfully completed.Predictions of the PEP model are superior to those of the stochastic model and result in a considerable reduction in computational time. Reproducibility of the results is an added advantage of the present formulation over the conventional stochastic simulations with random number generation. Given the possibility of analytical determination of the gas-particle velocity correlation coefficient still better predictions will be achievable with the present formulation.

References

1. Crowe,C.T., Sharma,M.P., and Stock,D.E., "The Particle-Source-in Cell (PSI-Cell) Model for Gas Droplet Flows",Journal of Fluid Engineering, (1977),pp. 275-332.

2. Gosman,A.D. and Ioannides,E.(1983). "Aspects of computer simulation of liquid fuelled combustors", Journal of Energy, Vol.7, No.6,p.482.

3. Hardalupas,Y.,Taylor,A.M.K.P., and Whitelaw,J.H.(1988), "Velocity and particle flux characteristics of turbulent particle laden jets",Imperial College, Mechanical Engineering Department, Fluids Section, Report FS/87/14.
4. Launder,B.E. and Spalding,D.B., The numerical computation of turbulent flows., Comp. Meth. Appl. Mech. and Eng., 3(1974), pp.269-289.
5. Lockwood,F.C. and Papadopoulos,C.(1989). "A new method for the computation of particulate dispersion in turbulent two-phase flows", Combustion and Flame, Vol 76, pp. 403-413.
6. Lumley,J.L. and Snyder,W.H.(1971), "Some measurements of particle velocity autocorrelation functions in a turbulent flow", Journal of Fluid Mechanics, Vol.48, p.41.
7. Morikawa,Y. and Tsuji,Y.(1982), "LDV measurements of an air-solid two-phase flow in a horizontal pipe", Journal of Fluid Mechanics, Vol.120, p. 385.
8. Papadopoulos,C.(1989), PhD Thesis, University of London.
9. Stock,D.E. and Wells,M.R.(1983), "The effects of crossing trajectories on the dispersion of particles in a turbulent flow", Journal of Fluid Mechanics, Vol.136, p. 31.

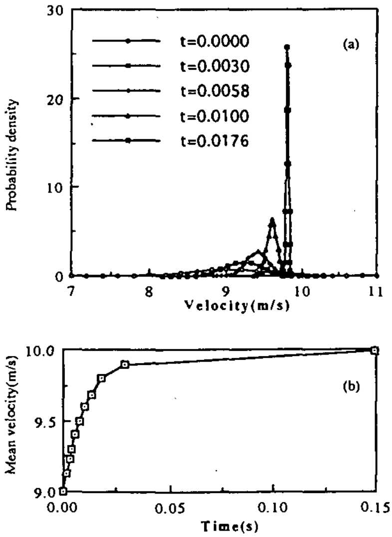

Figure 1: Particles of 40μm diameter in a uniform laminar flow, Gaussian velocity distribution at injection. (a) Evolution of velocity pdf in time , (b) mean velocity.

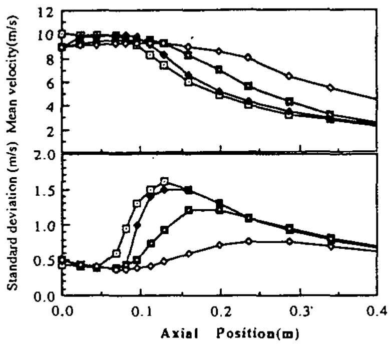

Figure 2: Response of particle phase to fully turbulent flow. Predictions using PEP model for particle diameters: 15μm, 40μm and 100μm . local gas velocity.

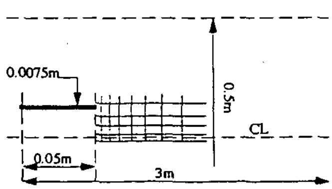

Figure 3: Computatinal domain. Nonuniform grid of 51*37

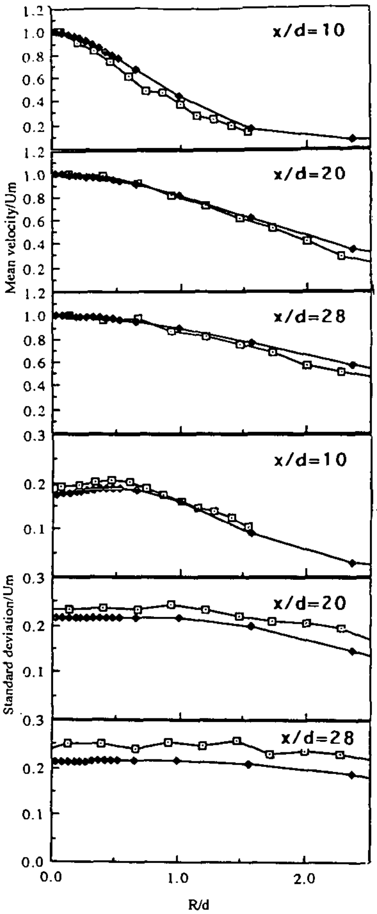

Figure 4: Predicted and measured radial profiles of mean axial velocity and standard deviation for single phase jet. -□- measurements, -◆- predictions. Results normalised by centreline axial velocity, Um.

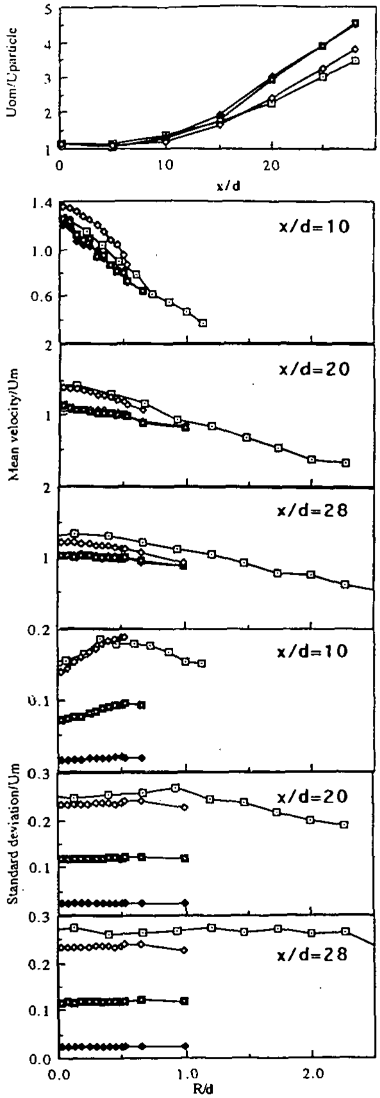

Figure 5: Predicted and measured mean axial velocity and standard deviation. (a) centreline profile, (b) radial profile [at three axial stations] for particle phase.□measurement. Predictions with velocity correlation coefficient -◇-1.0, -■-0.5 and -◆-0.1. Results normalised by centreline mean axial velocity,Um, and jet exit velocity,Uom, for clean jet.

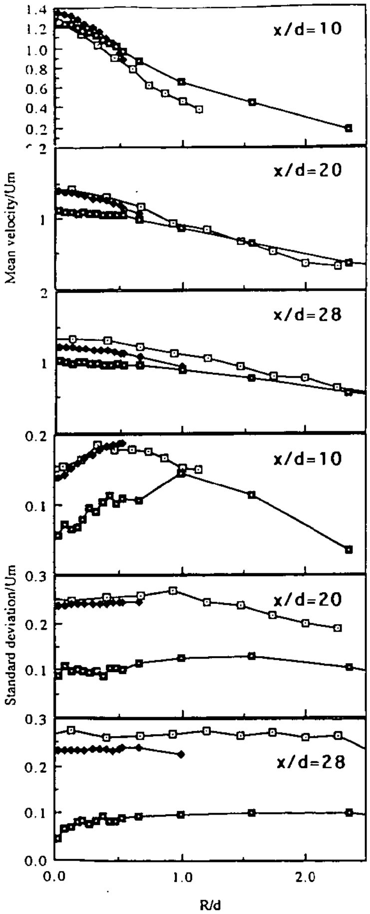

Figure 6: Predicted and measured radial profiles of mean axial velocity and standard deviation [at three axial stations] for particle phase. ⊡ measurement. Predictions: ◆ PEP model with ρgp=1.0, ◘ stochastic model. Results normalised by clean jet centre-line axial velocity, Um.

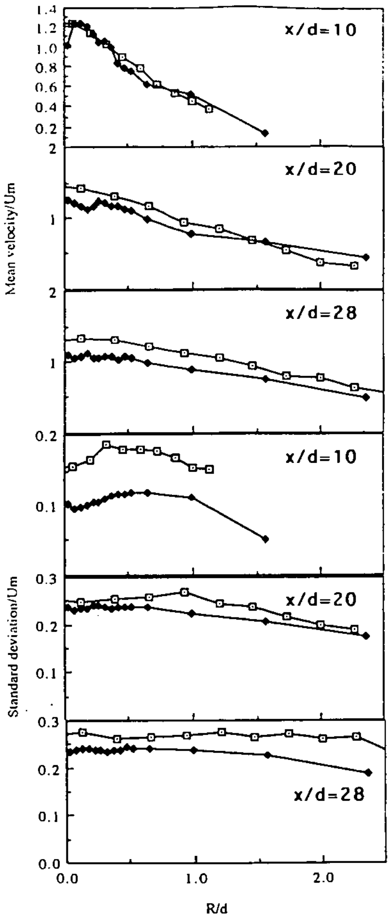

Figure 7: Predicted and measured radial profiles of mean axial velocity and standard deviation [at three axial stations for particle phase. ⊡ measurement. ◆ PEP model with a linearly varying velocity correlation coefficient. Results normalised by clean jet centreline axial velocity, Um.